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# MICROGRAM

## BULLETIN

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### SELECTED REFERENCES

The Selected References section is a compilation of recent publications of presumed interest to forensic chemists. Unless otherwise stated, all listed citations are published in English. Mailing address information duplicates that which is provided by the abstracting services.

Abdel-Hay KM, DeRuiter J, Randall Clark C. **GC-MS and GC-IRD studies on the six ring regioisomeric dimethoxybenzoylpiperazines (DMBzPs).** *Forensic Science International* 2013;231(1-3):54-60. [Editor's Notes: The compounds were not identified in the abstract. The perfluoroacyl derivatives of the regioisomers were resolved by GC and their mass spectra showed some differences in relative abundance of fragment ions, but without the appearance of any unique fragments. GC-IRD provides direct confirmatory data for the differentiation between the regioisomeric underivatized dimethoxybenzoylpiperazines. Contact: Department of Pharmacal Sciences, Harrison School of Pharmacy, Auburn University, Auburn, AL 36849.]

Cascini F, Passerotti S, Boschi I. **Analysis of THCA synthase gene expression in Cannabis: A preliminary study by real-time quantitative PCR.** *Forensic Science International* 2013;231(1-3):208-212. [Editor's Notes: The title study investigated a correlation between THC concentrations in Cannabis and the tetrahydrocannabinol acid synthase (THCAS) gene expression. Contact: Istituto di Sanita Pubblica, Sezione di Medicina Legale, Universita Cattolica del Sacro Cuore, Rome 00168, Italy.]

Cletus B, Olds W, Fredericks PM, Jaatinen E, Izake EL. **Real-time detection of concealed chemical hazards under ambient light conditions using Raman spectroscopy.** *Journal of Forensic Sciences* 2013;58(4):1008-1014. [Editor's Notes: Presents

a modified portable SORS sensor for detecting concealed substances in-field under different background lighting conditions. Applications include drugs (not detailed in the abstract). Contact: School of Chemistry, Physics and Mechanical Engineering, Science and Engineering Faculty, Queensland University of Technology, Brisbane QLD 4001, Australia.]

Deconinck E, Sacre P-Y, Courselle P, De Beer JO. **Chromatography in the detection and characterization of illegal pharmaceutical preparations.** *Journal of Chromatographic Science* 2013;51(8):791-806. [Editor's Notes: A review of the techniques used to characterize counterfeit and illegal pharmaceuticals, focusing on chromatographic techniques with different detection techniques. Contact: Division of Food, Medicines and Consumer Safety, Section Medicinal Products, Scientific Institute of Public Health (WIV-ISP), Brussels B-1050, Belgium.]

Demoranville LT, Brewer TM. **Ambient pressure thermal desorption ionization mass spectrometry for the analysis of substances of forensic interest.** *Analyst* 2013;138(18):5332-5337. [Editor's Notes: Presents the title technique. Tested substrates included several explosives and illicit drugs (not specified in the abstract). Very little or no sample prep is needed. Contact: Material Measurement Science Division, National Institute of Standards and Technology, MS-8371, 100 Bureau Dr., Gaithersburg, MD (zip code not provided).]

Dujourdy L, Csesztregi T, Bovens M, Franc A, Nagy J. **Sampling of illicit drugs for quantitative analysis. Part I: Heterogeneity study of illicit drugs in Europe.** *Forensic Science International* 2013;231(1-3):249-256. [Editor's Notes: It was determined that sampling problems caused by heterogeneity can be solved by using an incremental sampling protocol. This is stated

to be Part I of a planned 3 part study. Contact: Service Central des Laboratoires, Institut National de Police Scientifique, Ecully 69134, France.]

French HE, Went MJ, Gibson SJ. **Graphite furnace atomic absorption elemental analysis of ecstasy tablets.** *Forensic Science International* 2013;231(1-3):88-91. [Editor's Notes: Copper, magnesium, barium, nickel, chromium, and lead were determined in two separate batches of Ecstasy tablets; large intra-batch variations were found. Contact: School of Physical Sciences, University of Kent, Canterbury CT2 7NH, UK.]

Gaujac A, Martinez ST, Gomes AA, de Andrade SJ, da Cunha Pinto A, David JM, Navickiene S, Andrade JB. **Application of analytical methods for the structural characterization and purity assessment of N,N-dimethyltryptamine, a potent psychedelic agent isolated from Mimosa tenuiflora inner barks.** *Microchemical Journal* 2013;109:78-83. [Editor's Notes: Describes a simple, rapid method to isolate DMT from Mimosa tenuiflora. Includes characterization by FTIR, MS, MS/MS, 1H- and 13C-NMR, m.p., and UV. Contact: Instituto de Quimica, Universidade Federal da Bahia, 40170-115 Salvador, Brazil.]

Hoonka S, Durgbanshi A, Esteve-Romero J, Dubey NP, Bose D. **Simultaneous determination of three stupefacients in foodstuff using high performance liquid chromatography.** *Journal of Liquid Chromatography & Related Technologies* 2013, Ahead of Print. [Editor's Notes: PDA detection was used. The "stupefacients" were lidocaine, diazepam, and ketamine. Contact: Department of Criminology and Forensic Science, Dr. Harisingh Gour University, Sagar, India.]

Huang L, Yang X, Qi C, Niu X, Zhao C, Zhao X, Shangguan D, Yang Y. **A label-free electrochemical biosensor based on a DNA aptamer against codeine.** *Analytica Chimica Acta* 2013;787:203-

210. [Editor's Notes: The presented sensor exhibits high specificity to codeine over morphine. Contact: Chemistry and Chemical Engineering College, Yunnan Normal University, Kunming, Peoples Republic of China 650092.]

Hughes J, Ayoko G, Collett S, Golding G. **Rapid quantification of methamphetamine: Using Attenuated Total Reflectance Fourier Transform Infrared Spectroscopy (ATR-FTIR) and Chemometrics.** PLoS One 2013;8(7):e69609. [Editor's Notes: 96 samples were analyzed; the LOD was 7%. Contact: Discipline of Chemistry, Faculty of Science & Technology, Queensland University of Technology, Brisbane, Queensland, Australia.]

Lopez-Avila V, Zorio M. **Identification of methylhexanamine by GC high-resolution TOF-MS and soft ionization.** Forensic Science International 2013;231(1-3):113-119. [Editor's Notes: Derivatization with trifluoroacetic anhydride and analysis by the title technique differentiated methylhexanamine from the derivatives of 1-aminoheptane, 2-aminoheptane, 1,4-dimethylamylamine, and n-hexylmethylamine. Contact: Agilent Technologies, Santa Clara, CA 95051.]

Lu F, Weng X, Chai Y, Yang Y, Yu Y, Duan G. **A novel identification system for counterfeit drugs based on portable Raman spectroscopy.** Chemometrics and Intelligent Laboratory Systems 2013;127:63-69. [Editor's Notes: Focus is on counterfeit pharmaceuticals. Contact: School of Pharmacy, Fudan University, Shanghai 201203, Peoples Rep. China.]

Lurie IS, Driscoll SE, Cathapermal SS, Panicker S. **Determination of heroin and basic impurities for drug profiling by ultra-high-pressure liquid chromatography.** Forensic Science International 2013;231(1-3):300-305. [Editor's Notes: UHPLC enables enhanced analysis of heroin, morphine, O3- and O6-monoacetylmorphines, codeine, acetylcodeine, noscapine, and papaverine. Contact: Special Testing and Research Laboratory, U.S. Drug Enforcement Administration, Dulles, VA 20166.]

Maldaner AO, Schmidt LL, Locatelli MAF, Jardim WF, Sodre FF, Almeida FV, Pereira CEB, Silva CM. **Estimating cocaine consumption in the Brazilian Federal District (FD) by sewage analysis.** Journal of the Brazilian Chemical Society 2012;23(5):861-867. [Editor's Notes: The analytical methodology was not detailed in the abstract. Contact: Departamento de Policia Federal, Instituto Nacional de Criminalistica, 70610-200 Brasilia, DF, Brazil.]

Masetto de Gaitani C, De Oliveira ARM, Bonato PS. **Capillary electromigration techniques for the analysis of drugs and metabolites in biological matrices: A critical appraisal.** Capillary Electrophoresis and Microchip Capillary Electrophoresis 2013;229-245. [Editor's Notes: A review on strategies to obtain reliable capillary electromigration methods for the analysis of drugs and metabolites, including CE, CEC, and CE on microchips. Selectivity, detectability, efficiency, sample prepn., detectors, and repeatability are discussed. Selected applications are presented. Contact: Department of Pharmaceutical Sciences, University of Sao Paulo, Sao Paulo, Brazil.)

Mazina J, Alekseev V, Ivkina T, Kaljurand M, Poryvkina L. **Qualitative detection of illegal drugs (cocaine, heroin and MDMA) in seized street samples based on SFS data and ANN: Validation of method.** Journal of Chemometrics 2012;26(8-9):442-455. [Editor's Notes: Presents a spectral fluorescence signature (SFS) method combined with multilayer perceptron artificial neural networks (MLP-ANNs) for detection of the title drugs. Contact: Tallinn University of Technology/NarTest AS, Tallinn, Estonia.]

McKenzie EJ, Miskelly GM, Butler PAG. **Dynamic solid phase microextraction analysis for airborne methamphetamine: Quantitation using isotopically substituted methamphetamine.** Analytical Methods 2013;5(17):4391-4396. [Editor's Notes: Analysis by GC/MS. The results demonstrate that SPME can be used with pre-loaded isotopically substituted methamphetamine as an internal standard for accurate quantitation of airborne methamphetamine. Contact: Forensic Science Programme, School of Chemical Sciences, The University of Auckland, Auckland, N. Z.]

NicDaeid N, Jayaram S, Kerr WJ. **Elemental profiling using ICPMS of methylamphetamine hydrochloride prepared from proprietary medication using the Moscow and hypophosphorous synthesis.** Science & Justice 2013;53(3):278-285. [Editor's Notes: Presents and interprets inorganic profiles to determine within and between batch variations in known provenance samples produced via two different synthetic routes. The presence or absence of elements in the final synthesized products could be linked to the synthesis route, salting out method, and potentially the solvent used in the precursor extraction process. Contact: Centre for Forensic Science, Department of Pure and Applied Chemistry, WestCHEM, University of Strathclyde,

Pagano B, Lauri I, De Tito S, Persico G, Chini MG, Malmendal A, Novellino E, Randazzo A. **Use of NMR in profiling of cocaine seizures.** Forensic Science International 2013;231(1-3):120-124. [Editor's Notes: Presents the title study, as applied to samples seized at (unspecified) different times and places in Naples, Italy. Contact: Department of Pharmacy, University of Naples "Federico II", Naples 80131, Italy.]

Pascual Aguilar JA, Andreu V, Vazquez P, Pico Y. **Presence and spatial distribution of emerging contaminants (drugs of abuse) in protected agroecological systems (L'Albufera de Valencia Coastal Wetland, Spain).** Environmental Earth Sciences 2013, Ahead of Print. [Editor's Notes: The study focused on identifying the presence, flow paths, and spatial distribution of illicit drugs entering the title Natural Park. Analyses were conducted by LC/MS. Contact: Soil Degradation and Conservation Department, CIDE Desertification Research Centre, Valencia 46115, Spain.]

Qian Z-h, Xu P, Liu K-l. **New drug of designer cathinones "Bath Salts."** Zhongguo Yaowu Lanyong Fangzhi Zazhi 2013;19(1):42-44. [Editor's Notes: An overview and review. This article is written in Chinese. Contact: Institute of Forensic Science, Public Security Ministry, Beijing 100038, Peoples Republic of China.]

Rameev B, Mozzhukhin G, Aktas B. **Magnetic resonance detection of explosives and illicit materials.** Applied Magnetic Resonance 2012;43(4):463-467. [Editor's Notes: A review of the use of nuclear quadrupole and magnetic resonance (NQR and NMR) methods for detection of various solid-state and liquid explosive materials, illicit substances, and medicinal counterfeits. Contact: Gebze Institute of Technology, Gebze-Kocaeli, Turkey.]

Sekula K, Zuba D. **Structural elucidation and identification of a new derivative of phenethylamine using quadrupole time-of-flight mass spectrometry.** Rapid Communications in Mass Spectrometry 2013;27(18):2081-2090. [Editor's Notes: Presents characterization of 25I-NBMD [2-(4-iodo-2,5-dimethoxyphenyl)-N-[(2,3-methylenedioxyphenyl)methyl]ethanamine] by LC-ESI-QTOF-MS, GC/MS, and MS/MS. Contact: Institute of Forensic Research, Westerplatte 9, Krakow 31033, Poland.]

Thevis M, Volmer DA. **Recent instrumental progress in mass spectrometry: Advancing resolution,**

**accuracy, and speed of drug detection.** Drug Testing and Analysis 2012;4(3-4):242-245. [Editor's Notes: A review, covering the use of state-of-the-art mass spectrometers and recent instrumental developments such as new and/or improved hybrid analyzers. Contact: German Sport University Cologne, Institute of Biochemistry - Center for Preventive Doping Research, 50933 Cologne, Germany.]

Trzybinski D, Niedzialkowski P, Ossowski T, Trynda A, Sikorski A. **Single-crystal X-ray diffraction analysis of designer drugs: Hydrochlorides of methaphedrone and pentadron.** Forensic Science International 2013, Ahead of Print. [Editor's Notes: The technique allows identification of new substances for which there are no reference standards. Contact: University of Gdansk, Faculty of Chemistry, J. Sobieskiego 18/19, Gdansk 80-952, Poland.]

Tsujikawa K, Kuwayama K, Kanamori T, Iwata YT, Inoue H. **Thermal degradation of alpha-pyrrolidinopentiophenone during injection in gas chromatography/mass spectrometry.** Forensic Science International 2013;231(1-3):296-299. [Editor's Notes: Examines the factors controlling the thermal decomposition of alpha-PVP on GC liners. The use of a new deactivated liner minimized decomposition, even for splitless injections. An enamine compound is proposed for the decomposition product. Contact: National Research Institute of Police Science 6-3-1 Kashiwanoha, Kashiwa, Chiba 277-0882, Japan.]

Uemura N, Fukaya H, Kanai C, Yoshida M, Nakajima J-i, Takahashi M, Suzuki J, Moriyasu T, Nakae D. **Identification of a synthetic cannabinoid A-836339 as a novel compound found in a product.** Forensic Toxicology 2013, Ahead of Print. [Editor's Notes: Presents characterization of N-[3-(2-methoxyethyl)-4,5-dimethyl-2(3H)-thiazolylidene]-2,2,3,3-tetramethylcyclopropanecarboxamide (A-836339) by LC/MS, GC/MS, high-res MS, NMR, and X-ray crystallography. Contact: Tokyo Metropolitan Institute of Public Health, Shinjuku-ku, Tokyo 169-0073, Japan.]

Westwell AD, Hutchings A, Caldicott DGE. **The identification and chemical characterization of a new arylcyclohexylamine, methoxetamine, using a novel emergency department toxicosurveillance**

**tool.** Drug Testing and Analysis 2013;5(3):203-207. [Editor's Notes: Analysis by GC/MS, and <sup>1</sup>H- and <sup>13</sup>C-NMR. Contact: Cardiff School of Pharmacy and Pharmaceutical Sciences, Cardiff University, Cardiff, Wales, UK.]

Wong CHF, Ho ENM, Kwok WH, Leung DKK, Leung GNW, Tang FPW, Wong ASY, Wong JKY, Yu NH, Wan TSM. **Interconversion of ephedrine and pseudoephedrine during chemical derivatization.** Drug Testing and Analysis 2012;4(12):1028-1033. [Editor's Notes: Derivatization of ephedrine/pseudoephedrine with heptafluorobutyric anhydride was found to result in variable diastereomeric interconversion; the authors claim that this conversion has never been previously reported. Analyses were conducted by GC/MS. Toxicological focus. Contact: The Hong Kong Jockey Club, Sha Tin Racecourse, Sha Tin, Racing Laboratory, Hong Kong, Peop. Rep. China.]

Zawilska JB, Wojcieszak J. **Designer cathinones – An emerging class of novel recreational drugs.** Forensic Science International 2013;231(1-3):42-53. [Editor's Notes: An overview and review (abstract mentions mephedrone and MDPV). Contact: Department of Pharmacodynamics, Medical University of Lodz, Lodz 90-151, Poland.]

Zhai W-f, Zhang C-s, Gao L-s. **Study on determination of delta-9-tetrahydrocannabinol in Cannabis by high performance liquid chromatography.** Fenxi Ceshi Xuebao 2012;31(11):1379-1384. [Editor's Notes: Presents the title study. This article is written in Chinese. Contact: Department of Criminal Science and Technology, Chinese People's Public Security University, Beijing 100038, Peoples Republic of China.]

#### Additional References of Possible Interest

Boatto G, Pirisi MA, Burrai L, Baralla E, Demontis MP, Varoni MV, Nieddu M. **An LC-MS-MS method for quantitation of four new phenethylamines (BOX series) in plasma: In vivo application.** Forensic Toxicology 2013, Ahead of Print. [Editor's Notes: Analyses by LC-MS/MS. The four compounds were: 4-Bromo-2,5-beta-trimethoxyphenethylamine (BOB), 4-methyl-2,5-beta-trimethoxyphenethylamine (BOD), 3,4-methylenedioxy-beta-methoxyphenethylamine (BOH), and 4-methyl-2,5-dimethoxy-beta-

hydroxyphenethylamine (BOHD). Toxicological focus. Contact: Dipartimento di Chimica e Farmacia, Universita di Sassari, Sassari 07100, Italy.]

Chen C, Kostakis C, Irvine RJ, White JM. **Increases in use of novel synthetic stimulant are not directly linked to decreased use of 3,4-methylenedioxy-N-methylamphetamine (MDMA).** Forensic Science International 2013;231(1-3):278-283. [Editor's Notes: Wastewater samples were obtained from multiple treatment plants in Adelaide, Australia from 2009 to 2011, and analyzed by SPE-LC-MS/MS. The target compounds were: MDMA, mephedrone, methylone, MDPV, BZP, TFMPP, and methcathinone. The lag time from the decrease in MDMA to the increase in use of the other stimulants, indicated that there was no direct response to the reduction in MDMA use. Contact: Discipline of Pharmacology, School of Medical Sciences, The University of Adelaide, Australia.]

Eiler JM. **The isotopic anatomies of molecules and minerals.** Annual Review of Earth and Planetary Sciences 2013;41:411-441. [Editor's Notes: A review, describing the principles, background, analytical methodologies, existing tools, and likely future progress in this emerging field. Contact: Division of Geological and Planetary Sciences, California Institute of Technology, Pasadena, CA 91125.]

Fenech C, Nolan K, Rock L, Morrissey A. **An SPE LC-MS/MS method for the analysis of human and veterinary chemical markers within surface waters: An environmental forensics application.** Environmental Pollution 2013;181:250-256. [Editor's Notes: The use of co-occurring discriminators was assessed as a means to disentangle sewage and manure sources. Analyses were conducted by SPE-LC-MS/MS. Contact: School of Biotechnology, Dublin City University, Dublin, Ireland.]

Lee E-S, Lee JH, Han KM, Kim JW, Hwang IS, Cho S, Han SY, Kim J. **Simultaneous determination of 38 phosphodiesterase-5 inhibitors in illicit erectile dysfunction products by liquid chromatography-electrospray ionization-tandem mass spectrometry.** Journal of Pharmaceutical and Biomedical Analysis 2013;83:171-178. [Editor's Notes: Describes the development and validation of a



simultaneous analysis method for 38 compounds, including sildenafil, tadalafil, vardenafil and their analogs, in illicit erectile dysfunction products, by LC-ESI-MS/MS. Contact: Advanced Analysis Team, Toxicological Evaluation and Research Department, National Institute of Food and Drug Safety Evaluation, Korea Food & Drug Administration, Osong Health Technology Administration Complex, National Institute of Food and Drug Safety Evaluation, Chungcheongbuk-do, 363-700 S. Korea.]

Murray, Raymond C. **Forensic examination of soils.** Forensic Chemistry Handbook 2012, 109-130. Edited by Kobilinsky, Lawrence. John Wiley & Sons, Inc.: Hoboken, NJ. [Editor's Notes: A review. Contact: University of Montana, Missoula, MT.]

Parsons SM. **Date-rape drugs with emphasis on GHB.** Forensic Chemistry Handbook 2012, 355-434. Edited by Kobilinsky, Lawrence. John Wiley & Sons, Inc.: Hoboken, NJ. [Editor's Notes: A review. The date-rape drugs gamma-hydroxybutyrate (GHB), 3,4-methylenedioxymethamphetamine, flunitrazepam, and ketamine are discussed, with an emphasis on GHB. Contact: Department of Chemistry and Biochemistry, Program in Biomolecular and Engineering, Neuroscience Research Institute, University of California, Santa Barbara, CA.]

**Stable Isotope Forensics: An Introduction to the Forensic Application of Stable Isotope Analysis.**

2011, 296 pages. Edited by Meier-Augenstein, Wolfram. Wiley-Blackwell: Ames, IA.

Sundstroem M, Pelander A, Angerer V, Hutter M, Kneisel S, Ojanperae I. **A high-sensitivity ultra-high performance liquid chromatography/high-resolution time-of-flight mass spectrometry (UHPLC-HR-TOFMS) method for screening synthetic cannabinoids and other drugs of abuse in urine.** Analytical and Bioanalytical Chemistry 2013, Ahead of Print. [Editor's Notes: Toxicological focus. The database consisted of 277 compounds. Contact: Forensic Toxicology Division, Department of Forensic Medicine, Hjelt Institute, University of Helsinki, Helsinki 00014, Finland.]